



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:33 am BST

PDB ID : 5WBL
Title : Crystal structure of the Arabidopsis thaliana Raptor in complex with the TOS peptide of human PRAS40
Authors : Pavletich, N.P.; Jiang, X.
Deposited on : 2017-06-29
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

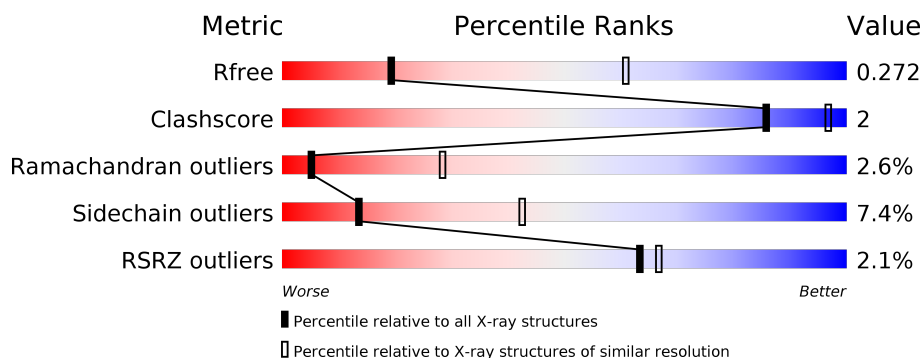
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1287	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> % 71% 9% 18% </div> </div>
2	T	16	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 19% 44% 6% 50% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8332 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Regulatory-associated protein of TOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1053	Total	C	N	O	S	0	0	0
			8273	5296	1420	1515	42			

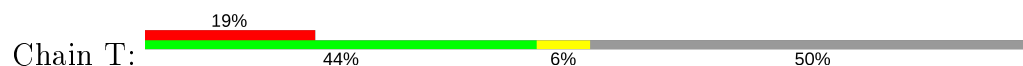
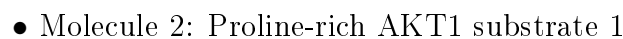
There are 3 discrepancies between the modelled and reference sequences:

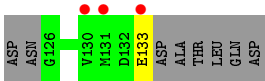
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q93YQ1
A	-1	VAL	-	expression tag	UNP Q93YQ1
A	0	ASP	-	expression tag	UNP Q93YQ1

- Molecule 2 is a protein called Proline-rich AKT1 substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	8	Total	C	N	O	S	0	0	0
			59	38	8	12	1			

- Molecule 1: Regulatory-associated protein of TOR 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.10Å 113.10Å 151.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.35 63.56 – 3.32	Depositor EDS
% Data completeness (in resolution range)	89.5 (20.00-3.35) 88.9 (63.56-3.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.205 , 0.266 0.215 , 0.272	Depositor DCC
R_{free} test set	898 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8332	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/8463	0.68	2/11496 (0.0%)
2	T	0.59	0/59	0.62	0/77
All	All	0.41	0/8522	0.68	2/11573 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	401	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	425	PRO	N-CA-CB	5.57	109.98	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1212	PRO	Peptide
1	A	1235	SER	Peptide
1	A	399	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8273	0	8274	37	0
2	T	59	0	53	0	0
All	All	8332	0	8327	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:GLN:O	1:A:1110:GLN:NE2	2.26	0.69
1:A:87:LEU:HD22	1:A:965:THR:HB	1.79	0.64
1:A:1163:ARG:NH2	1:A:1202:SER:O	2.32	0.59
1:A:408:HIS:CG	1:A:408:HIS:O	2.56	0.58
1:A:1223:SER:O	1:A:1234:VAL:HG23	2.06	0.56
1:A:1211:ARG:N	1:A:1212:PRO:HD2	2.21	0.55
1:A:158:GLN:HB3	1:A:301:THR:HG23	1.92	0.49
1:A:158:GLN:HB3	1:A:301:THR:CG2	2.42	0.49
1:A:1311:SER:O	1:A:1313:SER:N	2.46	0.49
1:A:277:ALA:HB3	1:A:396:ILE:HD12	1.96	0.48
1:A:575:VAL:HG13	1:A:582:GLN:HG2	1.95	0.48
1:A:1155:ASP:HB2	1:A:1162:VAL:HG21	1.96	0.47
1:A:237:THR:HB	1:A:238:PRO:HD3	1.95	0.47
1:A:469:LEU:HD13	1:A:502:VAL:HG12	1.97	0.47
1:A:1222:LEU:HB2	1:A:1234:VAL:HG22	1.96	0.46
1:A:1077:LYS:HB2	1:A:1092:ALA:HB3	1.97	0.46
1:A:1051:ILE:HB	1:A:1065:PHE:HB2	1.97	0.46
1:A:1063:ASN:ND2	1:A:1106:THR:O	2.49	0.45
1:A:655:ARG:NH2	1:A:1158:LYS:O	2.45	0.45
1:A:134:GLU:HA	1:A:294:ASP:HB2	2.00	0.44
1:A:1234:VAL:CG1	1:A:1235:SER:N	2.82	0.43
1:A:297:THR:O	1:A:301:THR:HB	2.19	0.43
1:A:142:MET:O	1:A:143:ALA:HB3	2.19	0.42
1:A:1211:ARG:O	1:A:1212:PRO:O	2.37	0.42
1:A:78:HIS:HB3	1:A:1113:VAL:HG13	2.01	0.42
1:A:249:ARG:HG2	1:A:396:ILE:HD11	2.02	0.42
1:A:698:LEU:HA	1:A:701:VAL:HG23	2.01	0.42
1:A:85:ALA:O	1:A:86:PRO:C	2.58	0.42
1:A:241:TYR:HB2	1:A:275:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ALA:HB2	1:A:858:VAL:HG22	2.02	0.41
1:A:538:GLN:NE2	1:A:576:ASP:O	2.51	0.41
1:A:1058:GLU:HB2	1:A:1060:THR:HG22	2.01	0.41
1:A:444:GLN:HG2	1:A:467:ILE:HD13	2.03	0.41
1:A:1081:ILE:HD11	1:A:1090:LEU:HD12	2.03	0.41
1:A:199:TYR:CZ	1:A:213:ILE:HG23	2.56	0.41
1:A:228:ILE:HG22	1:A:258:LEU:HD11	2.03	0.40
1:A:1242:ILE:HD11	1:A:1278:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1037/1287 (81%)	921 (89%)	89 (9%)	27 (3%)	5	28
2	T	6/16 (38%)	4 (67%)	2 (33%)	0	100	100
All	All	1043/1303 (80%)	925 (89%)	91 (9%)	27 (3%)	5	28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	LYS
1	A	685	GLU
1	A	1212	PRO
1	A	1213	HIS
1	A	1234	VAL
1	A	86	PRO
1	A	237	THR
1	A	409	MET
1	A	1086	ASP
1	A	1294	GLN

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Mol	Chain	Res	Type
1	A	1312	VAL
1	A	270	SER
1	A	1254	TYR
1	A	401	LEU
1	A	440	PHE
1	A	538	GLN
1	A	560	PHE
1	A	576	ASP
1	A	976	LYS
1	A	1067	ASN
1	A	1108	GLY
1	A	1119	ILE
1	A	1233	VAL
1	A	191	LYS
1	A	143	ALA
1	A	268	GLY
1	A	460	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	901/1097 (82%)	835 (93%)	66 (7%)	14	43
2	T	6/13 (46%)	5 (83%)	1 (17%)	2	9
All	All	907/1110 (82%)	840 (93%)	67 (7%)	13	42

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	87	LEU
1	A	94	LEU
1	A	100	LEU
1	A	103	ARG
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	118	THR
1	A	123	ASP
1	A	134	GLU
1	A	150	THR
1	A	161	ARG
1	A	165	ARG
1	A	175	THR
1	A	182	LEU
1	A	215	VAL
1	A	273	CYS
1	A	280	ASP
1	A	301	THR
1	A	320	ILE
1	A	321	ILE
1	A	332	ARG
1	A	344	ASN
1	A	396	ILE
1	A	408	HIS
1	A	415	MET
1	A	465	LEU
1	A	480	ARG
1	A	504	ILE
1	A	510	LYS
1	A	522	ILE
1	A	544	ASP
1	A	560	PHE
1	A	580	ARG
1	A	586	LEU
1	A	589	ASN
1	A	599	GLU
1	A	610	PRO
1	A	624	TRP
1	A	667	ASP
1	A	716	LEU
1	A	843	LEU
1	A	860	SER
1	A	958	ARG
1	A	1014	LEU
1	A	1016	ASN
1	A	1025	ARG
1	A	1048	ASN
1	A	1068	HIS

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Mol	Chain	Res	Type
1	A	1110	GLN
1	A	1111	LYS
1	A	1145	SER
1	A	1148	THR
1	A	1163	ARG
1	A	1164	SER
1	A	1180	GLN
1	A	1200	VAL
1	A	1212	PRO
1	A	1220	VAL
1	A	1222	LEU
1	A	1250	THR
1	A	1289	SER
1	A	1293	GLU
1	A	1300	TYR
1	A	1311	SER
1	A	1314	CYS
1	A	1323	LEU
2	T	133	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	A	357	ASN
1	A	835	GLN
1	A	1180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1053/1287 (81%)	0.12	19 (1%) 68 71	60, 109, 168, 248	0
2	T	8/16 (50%)	1.49	3 (37%) 0 0	140, 148, 159, 172	0
All	All	1061/1303 (81%)	0.13	22 (2%) 63 67	60, 109, 168, 248	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	ASP	13.1
1	A	683	ASP	9.6
1	A	680	GLU	9.4
1	A	1310	GLY	7.4
1	A	681	PHE	6.3
1	A	319	GLU	4.9
1	A	1311	SER	4.3
2	T	131	MET	3.0
1	A	1233	VAL	2.7
1	A	318	LYS	2.7
1	A	433	THR	2.5
1	A	1334	SER	2.5
2	T	133	GLU	2.4
2	T	130	VAL	2.4
1	A	317	LEU	2.3
1	A	686	LYS	2.3
1	A	264	SER	2.3
1	A	320	ILE	2.2
1	A	727	LEU	2.2
1	A	404	THR	2.1
1	A	88	GLY	2.0
1	A	514	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.